Phosphoric acid, 2-chloroethenyl diethyl ester
311-47-7 | DTXSID3075385

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 3.52e-11 cm3/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 2.34e-01

Confidence level: 8.28e-01

Nearest Neighbors from the Training Set

Image not found
2-Furancarboxaldehyde, 5-methyl-
Measured: 5.10e-11
Predicted: 4.23e-11

Image not found
(2E)-2-Hexenal
Measured: 4.40e-11
Predicted: 4.31e-11

Image not found
n-Butoxyacetaldehyde
Measured: 2.06e-11
Predicted: 2.17e-11

Image not found
Furfural
Measured: 3.51e-11
Predicted: 5.73e-11